

Long term analysis of splitting methods for charged-particle dynamics

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Abstract

In this paper, we rigorously analyze the energy, momentum and magnetic moment behaviours of two splitting methods for solving charged-particle dynamics. The near-conservations of these invariants are given for the system under constant magnetic field or quadratic electric potential. By the approach named as backward error analysis, we derive the modified equations and modified invariants of the splitting methods and based on which, the near-conservations over long times are proved. Some numerical experiments are presented to demonstrate these long time behaviours.

Keywords: Splitting method, charged particle dynamics, backward error analysis, near conservations, long term analysis.

Mathematics Subject Classification (2010): 65L05, 65P10, 78A35, 78M25

1. Introduction

In this paper, we formulate and analyze two splitting methods for solving the charged-particle dynamics (CPD) which is described by

$$\ddot{x} = v \times B(x) + E(x), \quad x(0) = x_0, \quad v(0) = v_0, \quad t \geq 0, \quad (1)$$

with the position $x(t) \in \mathbb{R}^3$ and the velocity $v(t) := \dot{x}(t) \in \mathbb{R}^3$, where $B(x) = \nabla_x \times A(x) \in \mathbb{R}^3$ denoted by $(B_1(x), B_2(x), B_3(x))^T$ is a non-uniform magnetic field which is determined by the vector potential $A(x)$, and $E(x) = -\nabla_x U(x)$ is a given electric field generated by some scalar potential $U(x)$. Charged particle dynamics plays a fundamental role in plasma physics ([2]) and there has been a lot of effective numerical methods in recent years for solving this system. Boris algorithm [3] has been widely used in the simulation of magnetized plasma due to its excellent properties [28, 29]. Many other kinds of methods have also been developed and analyzed, such as splitting methods [21, 25], exponential integrators [11], asymptotically preserving methods [9, 10], filtered Boris algorithms [17], uniformly accurate methods [6–8] and so on.

On the other hand, in the past over three decades, structure-preserving algorithms have arisen in various fields of applied sciences. From the scientific computing point of view, it is conventional to require numerical methods to preserve the qualitative features of the true solution as much as possible

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when applied to a differential equation. For the system of CPD (1), we pay attention to three important invariants. With the Euclidean norm $|\cdot|$, the total energy is denoted by ([4, 36])

$$H(x, v) = \frac{1}{2} |v|^2 + U(x). \quad (2)$$

It is well known that the solution of (1) exactly conserves this energy. For the scalar and vector potentials, if they are assumed to satisfy the invariance properties

$$U(e^{\tau S} x) = U(x), \quad e^{-\tau S} A(e^{\tau S} x) = A(x), \quad \forall \tau \in \mathbb{R}, \quad (3)$$

the momentum

$$M(x, v) = (v + A(x))^T S x$$

is preserved by the solution of (1) ([12]), where S is a skew-symmetric matrix. Moreover, if we consider the system (1) under the constant magnetic field, i.e. $B(x) \equiv B$ and S satisfies $Sv = v \times B$, then $A(x) = -\frac{1}{2}x \times B$ and the momentum becomes $M(x, v) = v^T(x \times B) - \frac{1}{2}|x \times B|^2$. The third invariant is the following magnetic moment

$$I(x, v) = \frac{|v \times B(x)|^2}{2|B(x)|^3} = \frac{|v_\perp|^2}{2|B(x)|},$$

where $v_\perp := \frac{v \times B(x)}{|B(x)|}$ is orthogonal to $B(x)$. Based on the analysis of [1, 5, 27], it is known that this magnetic moment is an *adiabatic invariant*.

From the point of long time scientific computation, it is of great interest to investigate the long time behaviour of numerical methods. In order to get numerical methods with near/exact conservation of qualitative features of the CPD, various numerical methods have been formulated and analyzed. Broadly speaking, up to the present, four categories of structure-preserving algorithms for the CPD have been in the center of research: energy-preserving methods [4, 22–24, 30, 32, 34] to preserve the energy, volume-preserving schemes [19] to preserve the volume, symplectic algorithms [20, 31, 35, 37] to preserve the symplecticity and numerical methods [12–16, 33] with near conservation of qualitative features. Recently splitting methods have been considered for solving CPD [21, 24, 34] and energy-preserving splitting methods have been constructed. However, these publications focus on the analysis of the accuracy and energy-preserving property of splitting methods. It seems that the long-time analysis of classical splitting methods has not been considered and the behaviour of energy-preserving splitting methods concerning other structure-preserving aspects has not been investigated in the literature, such as the long-time numerical conservation of momentum and magnetic moment. *From the perspective of structure preserving algorithm, this is far from enough.* Motivated by this point, this paper applies backward error analysis for two splitting methods to gain insight into their long-term energy, momentum and magnetic moment performance.

The rest of the paper is organized as follows. In section 2, we describe two different symmetric splitting methods and study their local errors. Then, in section 3, the main results on the numerical long time conservation are presented and three numerical experiments are carried out to support the theoretical results. The complete analysis of the results are rigorously given in section 4. The last section is devoted to the conclusions of this paper.

2. Numerical Methods

In this section, we present two splitting methods and show their elementary features. To formulate the

methods, we split the equation (1) into two subflows:

$$\frac{d}{dt} \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} 0 \\ v \times B(x) \end{pmatrix}, \quad \frac{d}{dt} \begin{pmatrix} x \\ v \end{pmatrix} = \begin{pmatrix} v \\ E(x) \end{pmatrix}. \quad (4)$$

Then for the first subflow, which is integrable, one can obtain its exact solution:

$$\Phi_t^L : \begin{pmatrix} \xi(t) \\ \eta(t) \end{pmatrix} = \begin{pmatrix} \xi(0) \\ e^{t\tilde{B}(\xi(0))}\eta(0) \end{pmatrix}, \quad t \geq 0, \quad (5)$$

where $\tilde{B}(x) = \begin{pmatrix} 0 & B_3(x) & -B_2(x) \\ -B_3(x) & 0 & B_1(x) \\ B_2(x) & -B_1(x) & 0 \end{pmatrix}$ is defined by $v \times B(x) = \tilde{B}(x)v$. For the second subflow (a canonical Hamiltonian system), we consider applying the average vector field (AVF) formula [26] to get its numerical propagator:

$$\Phi_t^{iL} : \begin{pmatrix} \xi(t) \\ \eta(t) \end{pmatrix} = \begin{pmatrix} \xi(0) + t\eta(0) + \frac{t^2}{2} \int_0^1 E(\rho\xi(0) + (1-\rho)\xi(t)) d\rho \\ \eta(0) + t \int_0^1 E(\rho\xi(0) + (1-\rho)\xi(t)) d\rho \end{pmatrix}. \quad (6)$$

Based on this splitting, two methods are formulated as follows.

Algorithm 2.1 (Implicit splitting method). We denote the numerical solution as $x^n \approx x(t_n)$, $v^n \approx v(t_n)$ and choose $x^0 = x_0$, $v^0 = v_0$. Taking a symmetric version [18]: $\Phi_h^i = \Phi_{\frac{h}{2}}^L \circ \Phi_h^{iL} \circ \Phi_{\frac{h}{2}}^L$, then we get its total formula for solving (1): for $n \geq 0$,

$$\begin{aligned} x^{n+1} &= x^n + h e^{\frac{h}{2}\tilde{B}(x^n)} v^n + \frac{h^2}{2} \int_0^1 E(\rho x^n + (1-\rho)x^{n+1}) d\rho, \\ v^{n+1} &= e^{\frac{h}{2}(\tilde{B}(x^{n+1}) + \tilde{B}(x^n))} v^n + h e^{\frac{h}{2}\tilde{B}(x^{n+1})} \int_0^1 E(\rho x^n + (1-\rho)x^{n+1}) d\rho. \end{aligned} \quad (7)$$

Obviously, it is an implicit and typical Strang splitting scheme, and we shall use IMS-O2 to denote the method.

If we make some adjustments to (6), we can get the following explicit algorithm.

Algorithm 2.2 (Explicit splitting method). For the second subflow in (4), we linearize the nonlinear integrals in (6), and then it is transformed to

$$\Phi_t^{eL} : \begin{pmatrix} \xi(t) \\ \eta(t) \end{pmatrix} = \begin{pmatrix} \xi(0) + t\eta(0) + \frac{t^2}{2} E(\xi(0)) \\ \eta(0) + \frac{t}{2} [E(\xi(0)) + E(\xi(t))] \end{pmatrix}. \quad (8)$$

In that way, the Strang splitting scheme $\Phi_h^e := \Phi_{\frac{h}{2}}^L \circ \Phi_h^{eL} \circ \Phi_{\frac{h}{2}}^L$ for solving (1) reads:

$$\begin{aligned} x^{n+1} &= x^n + h e^{\frac{h}{2}\tilde{B}(x^n)} v^n + \frac{h^2}{2} E(x^n), \\ v^{n+1} &= e^{\frac{h}{2}(\tilde{B}(x^{n+1}) + \tilde{B}(x^n))} v^n + \frac{h}{2} e^{\frac{h}{2}\tilde{B}(x^{n+1})} [E(x^n) + E(x^{n+1})], \end{aligned} \quad (9)$$

and we shall call it as EXS-O2.

In what follows, we will study the basic properties of these two methods. We begin with their symmetry. A numerical method denoted by $y^{n+1} = \Phi_h(y^n)$ is called symmetric if exchanging $y^n \leftrightarrow y^{n+1}$ and $h \leftrightarrow -h$ leaves the method unaltered. It has been pointed out in [18] that symmetric methods have excellent long time behavior and play a central role in the geometric numerical integration of differential equations. The following theorem states the symmetry of Algorithms 2.1 and 2.2.

Theorem 2.3 (Symmetry). *From the symmetric versions: $\Phi_h^i = \Phi_{\frac{h}{2}}^L \circ \Phi_h^{iL} \circ \Phi_{\frac{h}{2}}^L$ and $\Phi_h^e = \Phi_{\frac{h}{2}}^L \circ \Phi_h^{eL} \circ \Phi_{\frac{h}{2}}^L$, it follows that Algorithms 2.1 and 2.2 are symmetric.*

For these two algorithms, we next investigate and briefly show their local errors.

Theorem 2.4 (Local errors). *For the two methods presented above, under the local assumptions $x(t_n) = x^n, v(t_n) = v^n$, the local errors are given as*

$$x^{n+1} - x(t_{n+1}) = O(h^3), \quad v^{n+1} - v(t_{n+1}) = O(h^3),$$

where the constants symbolized by O are independent of n and h .

Proof. For simplicity of notations, we denote

$$y := \begin{pmatrix} x \\ v \end{pmatrix}, \quad f(y) := \begin{pmatrix} v \\ v \times B(x) + E(x) \end{pmatrix}, \quad f_1(y) := \begin{pmatrix} 0 \\ v \times B(x) \end{pmatrix}, \quad f_2(y) = \begin{pmatrix} v \\ E(x) \end{pmatrix},$$

and let Φ_h stand for the exact flow. Then the original system can be rewritten as $\dot{y} = f(y) = f_1(y) + f_2(y)$.

By Taylor expansions, we reach

$$\begin{aligned} \Phi_h(y) &= \left[Id + hf + \frac{h^2}{2} f' f \right] (y) + O(h^3), & \Phi_h^L(y) &= \left[Id + hf_1 + \frac{h^2}{2} f'_1 f_1 \right] (y) + O(h^3), \\ \Phi_h^{iL}(y) &= \left[Id + hf_2 + \frac{h^2}{2} f'_2 f_2 \right] (y) + O(h^3), & \Phi_h^{eL}(y) &= \left[Id + hf_2 + \frac{h^2}{2} f'_2 f_2 \right] (y) + O(h^3). \end{aligned}$$

Note that $\Phi_h^{iL}(y) \neq \Phi_h^{eL}(y)$ due to their different coefficients of the term $O(h^3)$. After some calculations, we get

$$\begin{aligned} \Phi_h^i(y) &= \Phi_{\frac{h}{2}}^L \circ \Phi_h^{iL} \circ \Phi_{\frac{h}{2}}^L(y) = \left[Id + h(f_1 + f_2) + \frac{h^2}{2} (f'_1 f_1 + f'_1 f_2 + f'_2 f_1 + f'_2 f_2) \right] (y) + O(h^3) \\ &= \Phi_h(y) + O(h^3). \end{aligned}$$

Even if EXS-O2 is the linearization of IMS-O2, the expansions of Φ_h^{iL} and Φ_h^{eL} are similar. Hence, it can be verified that this makes no difference to the error result, i.e., $\Phi_h^e(y) - \Phi_h(y) = O(h^3)$. ■

3. Main results and numerical experiments

3.1. Main results

In this subsection, we assume that the scalar potential $U(x)$ and the magnetic field $B(x)$, as functions of x , are arbitrarily differentiable. In this paper, $B(x) \equiv B$ represents the constant magnetic field and $U(x) = \frac{1}{2} x^\top Q x + q^\top x$ with a symmetric matrix Q refers to the quadratic scalar potential. Meanwhile, it is assumed that there exists a compact set (independent of h) such that the result (x^n, v^n) produced by the considered method stays in this set. Then the energy, momentum and magnetic moment behaviours of Algorithms 2.1 and 2.2 are given as follows one by one.

Theorem 3.1 (Energy conservation). *The method IMS-O2 exactly preserves the energy (2) of CPD [24], i.e.*

$$\text{IMS} - \text{O2} : \quad H(x^n, v^n) = H(x^0, v^0) \quad \text{for} \quad nh \leq T.$$

We assume that $B(x) \equiv B$ or $U(x) = \frac{1}{2}x^\top Qx + q^\top x$, then the energy (2) along the numerical solution over long times is conserved as follows

$$\text{EXS} - \text{O2} : \quad H(x^n, v^n) = H(x^0, v^0) + O(h^2) \quad \text{for} \quad nh \leq h^{2-N}, \quad (10)$$

with an arbitrarily large positive integer N .

Moreover, the method EXS-O2 has an exact modified energy conservation which is stated as below. If the scalar potential $U(x)$ is quadratic, EXS-O2 (9) exactly preserves the modified energy

$$H_h(x, v) = \frac{1}{2} |v|^2 + U(x) - \frac{h^2}{8} |\nabla U(x)|^2 \quad (11)$$

at the discrete level, i.e.

$$\text{EXS} - \text{O2} : \quad H_h(x^{n+1}, v^{n+1}) = H_h(x^n, v^n) \quad \text{for} \quad nh \leq T. \quad (12)$$

Theorem 3.2 (Momentum conservation). *Under the conditions (3) and the following two assumptions:*

- $B(x) \equiv B$ and $Sv = v \times B$,
- $U(x) = \frac{1}{2}x^\top Qx + q^\top x$ and $QS = SQ$,

the momentum $M(x, v) = (v + A(x))^\top Sx$ along the numerical solution over long times is nearly preserved as

$$M(x^n, v^n) = M(x^0, v^0) + O(h^2) \quad \text{for} \quad nh \leq h^{2-N}, \quad (13)$$

where N is an arbitrarily large positive integer.

Theorem 3.3 (Magnetic moment conservation). *Assume that the following two assumptions hold:*

- $B(x) \equiv B$,
- $U(x) = \frac{1}{2}x^\top Qx + q^\top x$ and $Q\widehat{B} = \widehat{B}Q$ with $v \times \frac{B}{|B|} = \widehat{B}v$,

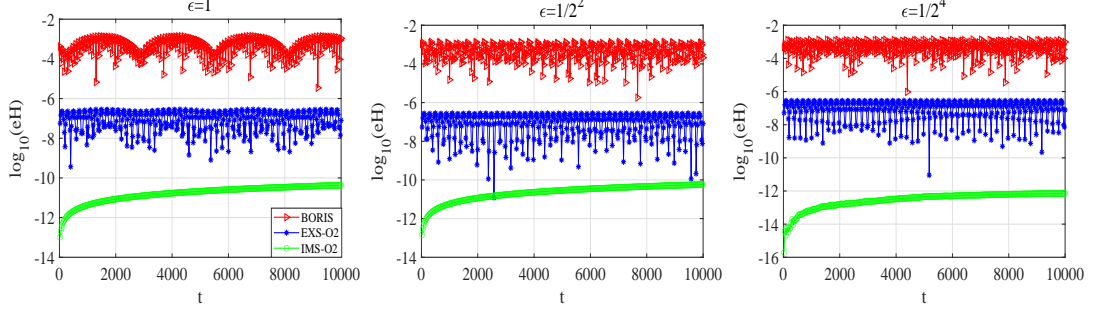
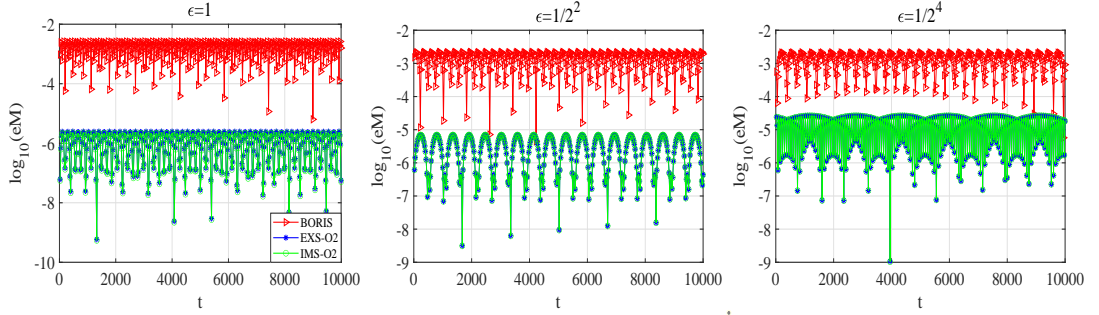
then the near conservation of magnetic moment $I(x, v)$ is

$$I(x^n, v^n) = I(x^0, v^0) + O(h^2) \quad \text{for} \quad nh \leq h^{2-N}, \quad (14)$$

with an arbitrarily large positive integer N .

3.2. Numerical experiments

In this part, by means of MATLAB, we present three numerical experiments to show the long time energy, momentum, and magnetic moment behaviour of the above splitting methods. We choose Boris method for comparison, and solve all the tests on $[0, 10000]$ with the step size $h = 0.01$ to show the long time conservations. For IMS-O2, the fixed-point iteration is employed into implicit iteration, where the error tolerance is 10^{-16} and the maximum number of each iteration is 50. In addition, we make use of

Figure 1: Problem 1. Evolution of the energy error e_H as function of time t .Figure 2: Problem 1. Evolution of the energy error e_M as function of time t .

Gauss-Legendre to deal with the nonlinear integral in (7). Denote the relative errors of energy, momentum and magnetic moment respectively by

$$e_H := \frac{|H(x^n, v^n) - H(x^0, v^0)|}{|H(x^0, v^0)|}, \quad e_M := \frac{|M(x^n, v^n) - M(x^0, v^0)|}{|M(x^0, v^0)|}, \quad e_I := \frac{|I(x^n, v^n) - I(x^0, v^0)|}{|I(x^0, v^0)|}. \quad (15)$$

For the momentum $M(x, v) = (v + A(x))^T S x$, throughout this subsection, the skew-symmetric matrix is given as $S = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$, i.e. $M(x, v) = (v_1 + A_1(x))x_2 - (v_2 + A_2(x))x_1$.

Problem 1. (Quadratic scalar potential and constant magnetic field) We first consider the charged particle dynamics (1) with the quadratic scalar potential $U(x) = \frac{x_1^2 + x_2^2 + x_3^2}{100}$ and the constant magnetic field $B = -\nabla \times \frac{1}{2\varepsilon}(x_2, -x_1, 0)^T = \frac{1}{\varepsilon}(0, 0, 1)^T$. Particularly when $\varepsilon = 1$, we have $\widehat{B} = \frac{\bar{B}}{|B|} = \bar{B} = S$ and $QS = SQ$. The initial values are chosen as $x(0) = (0, 1, 0.1)^T$ and $v(0) = (0.09, 0.05, 0.20)^T$. The errors in (15) are respectively displayed in Figs. 1–3. In addition, let $e_{H_h} := \frac{|H_h(x^n, v^n) - H_h(x^0, v^0)|}{|H_h(x^0, v^0)|}$ with H_h (11). The conservation of e_{H_h} by EXS-O2 is displayed in Fig. 4.

Problem 2. (Constant magnetic field) As the second problem, we consider a general scalar potential $U(x) = \frac{1}{100\sqrt{x_1^2 + x_2^2}}$. The magnetic field and the initial values are the same as those in Problem 1. The errors

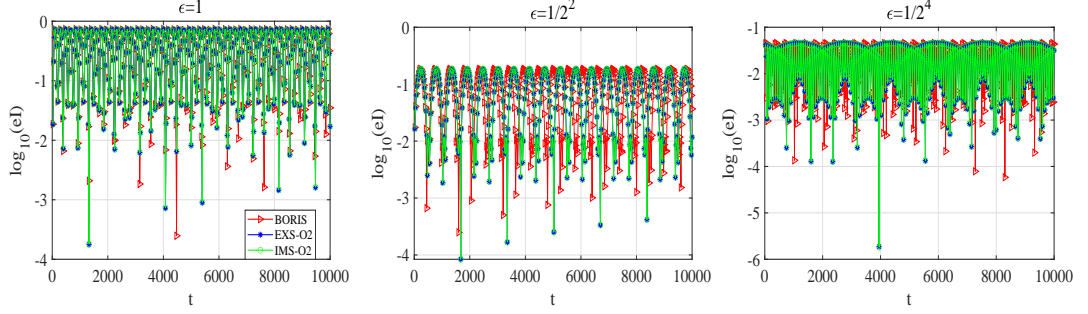


Figure 3: Problem 1. Evolution of the energy error e_I as function of time t .

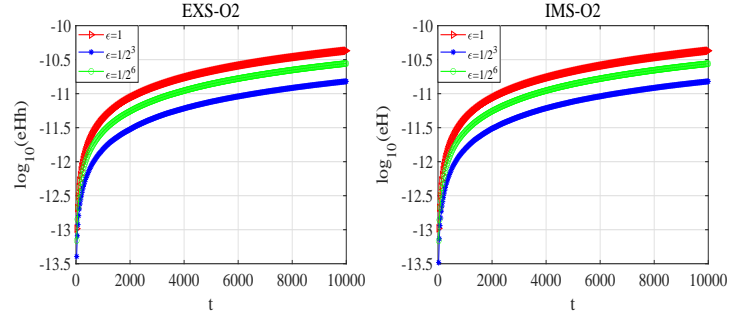


Figure 4: Problem 1. Evolution of the energy error e_{H_h} for EXS-O2 and e_H for IMS-O2 as functions of time t with $\varepsilon = 1, 1/2^3, 1/2^6$.

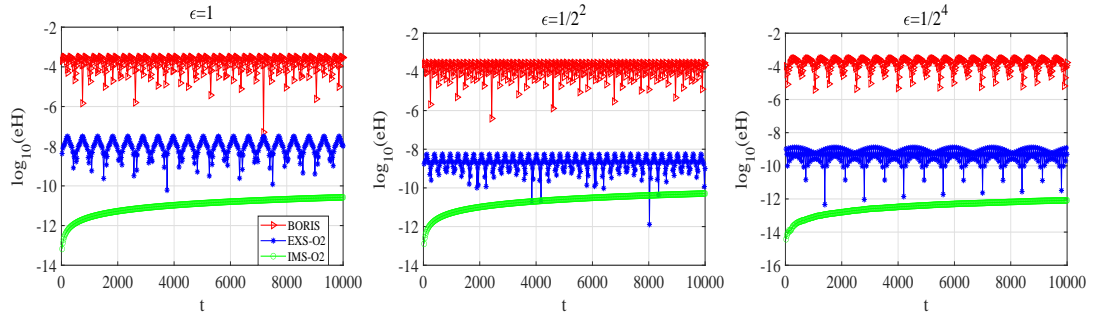


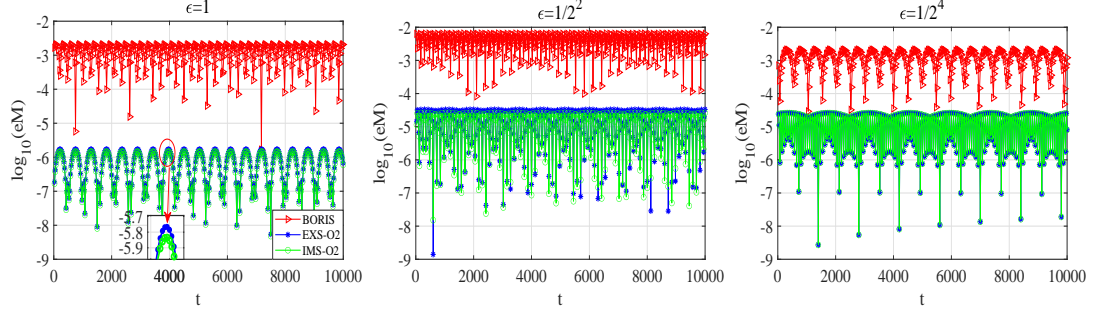
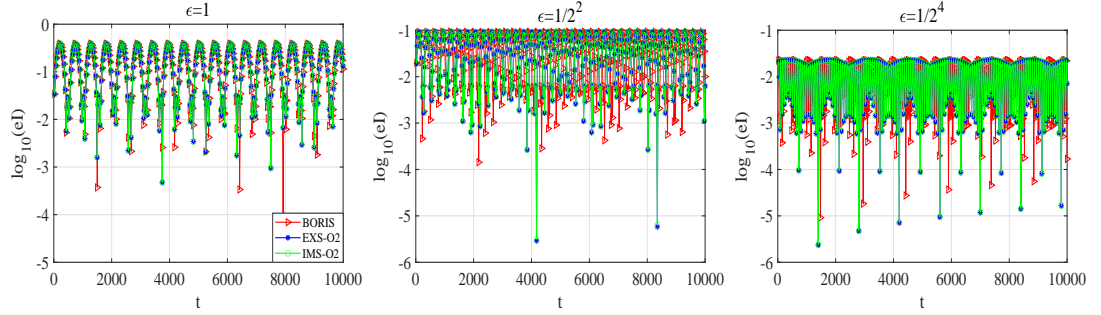
Figure 5: Problem 2. Evolution of the energy error e_H as function of time t .

in (15) are respectively presented in Figs. 5–7.

Problem 3. (General case) In the third numerical experiment, we are interested in a general case that the scalar potential is the same as it in Problem 2 and the magnetic field is

$$B(x) = \nabla \times \frac{1}{3\varepsilon} (-x_2 \sqrt{x_1^2 + x_2^2}, -x_1 \sqrt{x_1^2 + x_2^2}, 0)^T = \frac{1}{\varepsilon} (0, 0, \sqrt{x_1^2 + x_2^2})^T.$$

The initial values are the same as those in Problem 1. Then errors in (15) are severally shown in Figs.

Figure 6: Problem 2. Evolution of the energy error e_M as function of time t .Figure 7: Problem 2. Evolution of the energy error e_I as function of time t .

8–10. Besides, in order to show the accuracy of the methods, we plot the global errors $error := \frac{|x^n - x(t_n)|}{x(t_n)} + \frac{|v^n - v(t_n)|}{v(t_n)}$ at $t_{end} = 1$ in Fig 11, where the reference solution is obtained by using “ode45” of MATLAB.

In accordance with these numerical results, we have the following observations.

- **Energy conservation.** Clearly from Figs. 1, 5 and 8, we can see that only IMS-O2 is energy-preserving, Boris and EXS-O2 show a long-term energy behavior, and EXS-O2 behaves better than Boris. Meanwhile, Fig 4 demonstrates that EXS-O2 exactly preserves the energy H_h .

- **Momentum conservation.** In the light of the results given by Figs. 2, 6 and 9, all the three methods are not momentum-preserving but they hold a long time momentum conservation. Besides, the behaviour of our methods is better than the Boris algorithm.

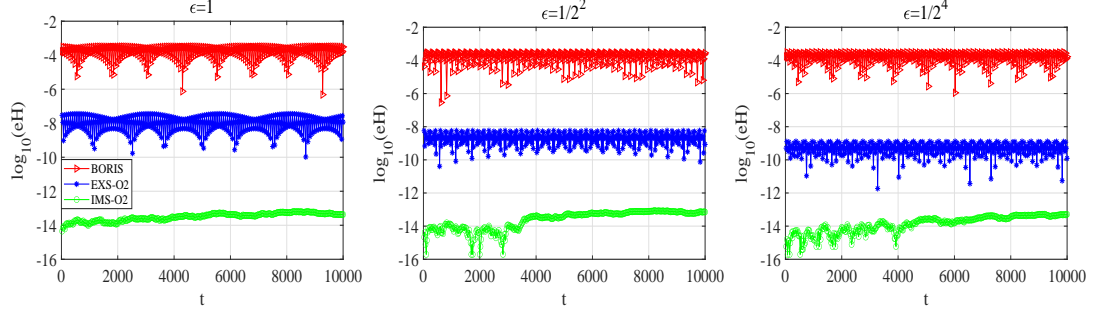
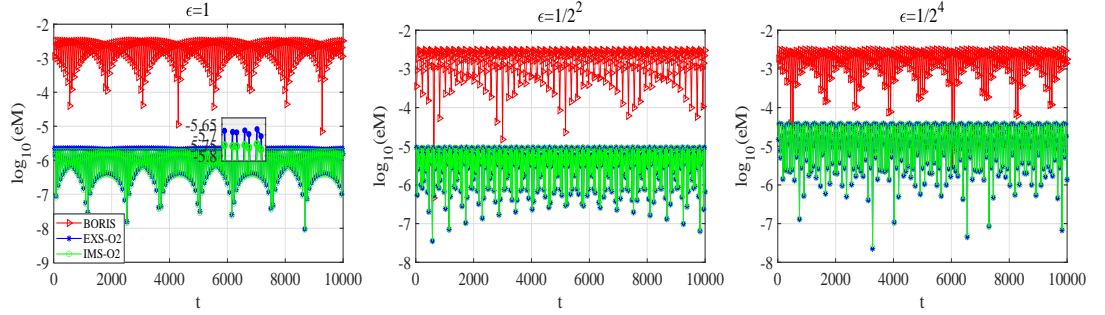
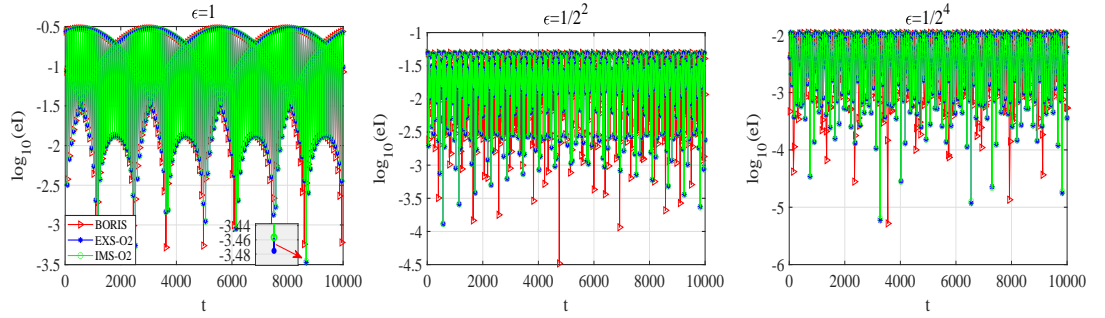
- **Magnetic Moment conservation.** Observing Figs. 3, 7 and 10, all the methods have similar magnetic moment conservations over long times.

- **Accuracy.** Fig. 11 confirms that our IMS-O2 and EXS-O2 both have second-order accuracy and they perform better than the Boris algorithm.

The numerical results of Problems 1 and 2 support the theoretical conclusions given in Section 3.1. It is noted that for the general system (Problem 3), the methods also show a long time conservation in the energy, momentum, and magnetic moment, which is more than expected.

4. Proofs of the main results

In this section, we rigorously prove the main results given in Section 3.1. The technical tool so called the backward error analysis [18] which is indispensable for the study of equations or numerical solutions

Figure 8: Problem 3. Evolution of the energy error e_H as function of time t .Figure 9: Problem 3. Evolution of the energy error e_M as function of time t .Figure 10: Problem 3. Evolution of the energy error e_I as function of time t .

over long times will be used in the following proofs.

4.1. Backward error analysis

Following the analysis of backward error analysis, the main idea is to find a modified differential equation whose solution $z(t)$ at $t = nh$ is equivalent to the numerical result x^n produced by the considered method.

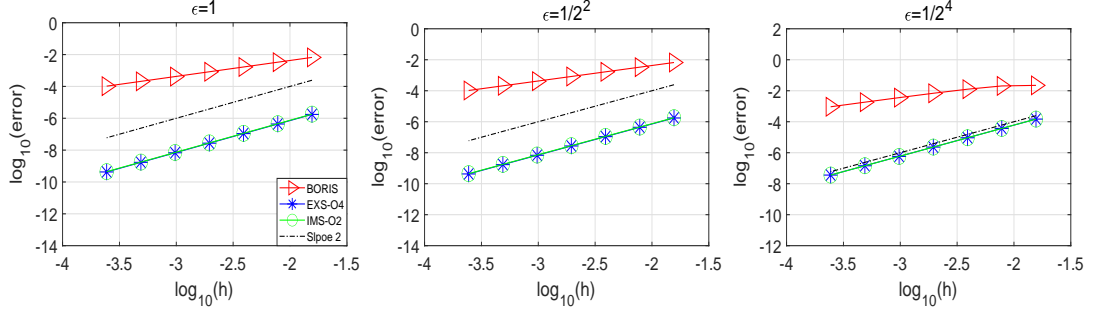


Figure 11: Problem 3. The global errors $error$ with $t = 1$ and $h = \frac{1}{2^k}$ for $k = 6, \dots, 12$ under different ε .

EXS-O2. On the basis of the first equation in (9) and the symmetry of EXS-O2, we get

$$x^{n-1} = x^n - h e^{-\frac{h}{2}\tilde{B}(x^n)} v^n + \frac{h^2}{2} E(x^n).$$

This result and the first one of (9) give

$$\begin{aligned} x^{n+1} - 2x^n + x^{n-1} &= h \left(e^{\frac{h}{2}\tilde{B}(x^n)} - e^{-\frac{h}{2}\tilde{B}(x^n)} \right) v^n + h^2 E(x^n), \\ x^{n+1} - x^{n-1} &= h \left(e^{\frac{h}{2}\tilde{B}(x^n)} + e^{-\frac{h}{2}\tilde{B}(x^n)} \right) v^n. \end{aligned}$$

Elimination of v^n leads to

$$\frac{x^{n+1} - 2x^n + x^{n-1}}{h^2} = \frac{2 e^{\frac{h}{2}\tilde{B}(x^n)} - e^{-\frac{h}{2}\tilde{B}(x^n)}}{h \left(e^{\frac{h}{2}\tilde{B}(x^n)} + e^{-\frac{h}{2}\tilde{B}(x^n)} \right)} \frac{x^{n+1} - x^{n-1}}{2h} + E(x^n).$$

According to the special scheme of $\tilde{B}(x)$, it is obtained that

$$\frac{2 e^{\frac{h}{2}\tilde{B}(x^n)} - e^{-\frac{h}{2}\tilde{B}(x^n)}}{h \left(e^{\frac{h}{2}\tilde{B}(x^n)} + e^{-\frac{h}{2}\tilde{B}(x^n)} \right)} = \frac{\tan\left(\frac{h}{2}|B(x^n)|\right)}{\frac{h}{2}|B(x^n)|} \tilde{B}(x^n),$$

and such that

$$\frac{x^{n+1} - 2x^n + x^{n-1}}{h^2} = \frac{\tan\left(\frac{h}{2}|B(x^n)|\right)}{\frac{h}{2}|B(x^n)|} \frac{x^{n+1} - x^{n-1}}{2h} \times B(x^n) + E(x^n).$$

For a fixed t , the function $z(t)$ has to satisfy

$$\frac{z(t+h) - 2z(t) + z(t-h)}{h^2} = \frac{\tan\left(\frac{h}{2}|B(z(t))|\right)}{\frac{h}{2}|B(z(t))|} \frac{z(t+h) - z(t-h)}{2h} \times B(z(t)) + E(z(t)).$$

We let $z := z(t)$ and expand the above functions in powers of h , so that

$$\ddot{z} + \frac{h^2}{12} \dddot{z} + \dots = \frac{\tan\left(\frac{h}{2}|B(z)|\right)}{\frac{h}{2}|B(z)|} \left(\dot{z} + \frac{h^2}{6} \ddot{z} + \dots \right) \times B(z) + E(z). \quad (16)$$

IMS-O2. In an analogous way, the scheme (7) of IMS-O2 can be formulated as

$$\begin{aligned}
& \frac{x^{n+1} - 2x^n + x^{n-1}}{h^2} \\
&= \frac{2}{h} \frac{e^{\frac{h}{2}\tilde{B}(x^n)} - e^{-\frac{h}{2}\tilde{B}(x^n)}}{e^{\frac{h}{2}\tilde{B}(x^n)} + e^{-\frac{h}{2}\tilde{B}(x^n)}} \tilde{B}(x^n) \left[\frac{x^{n+1} - x^{n-1}}{2h} - \frac{h}{4} \int_0^1 \left[E(\rho x^n + (1-\rho)x^{n+1}) - E(\rho x^n + (1-\rho)x^{n-1}) \right] d\rho \right] \\
& \quad + \frac{1}{2} \int_0^1 \left[E(\rho x^n + (1-\rho)x^{n+1}) + E(\rho x^n + (1-\rho)x^{n-1}) \right] d\rho \\
&= \frac{\tan\left(\frac{h}{2}|B(x^n)|\right)}{\frac{h}{2}|B(x^n)|} \left[\frac{x^{n+1} - x^{n-1}}{2h} - \frac{h}{4} \int_0^1 \left[E(x^n + \rho(x^{n+1} - x^n)) - E(x^n + \rho(x^{n-1} - x^n)) \right] d\rho \right] \times B(x^n) \\
& \quad + \frac{1}{2} \int_0^1 \left[E(x^n + \rho(x^{n+1} - x^n)) + E(x^n + \rho(x^{n-1} - x^n)) \right] d\rho \\
&= \frac{\tan\left(\frac{h}{2}|B(x^n)|\right)}{\frac{h}{2}|B(x^n)|} \left[\frac{x^{n+1} - x^{n-1}}{2h} - \left(\frac{h}{8} E'(x^n)(x^{n+1} - x^{n-1}) + \dots \right) \right] \times B(x^n) \\
& \quad + E(x^n) + \frac{1}{4} E'(x^n)(x^{n+1} - 2x^n + x^{n-1}) + \dots,
\end{aligned}$$

where the following fact is used here

$$\begin{aligned}
& \int_0^1 E(\rho x^n + (1-\rho)x^{n+1}) d\rho = \int_0^1 E(\rho x^{n+1} + (1-\rho)x^n) d\rho = \int_0^1 E(x^n + \rho(x^{n+1} - x^n)) d\rho \\
&= \int_0^1 \left[E(x^n) + E'(x^n)\rho(x^{n+1} - x^n) + \dots \right] d\rho = E(x^n) + \frac{1}{2} E'(x^n)(x^{n+1} - x^n) + \dots.
\end{aligned}$$

Therefore, the function $z(t)$ satisfies

$$\begin{aligned}
& \frac{z(t+h) - 2z(t) + z(t-h)}{h^2} \\
&= \frac{\tan\left(\frac{h}{2}|B(z(t))|\right)}{\frac{h}{2}|B(z(t))|} \left[\frac{z(t+h) - z(t-h)}{2h} - \left(\frac{h}{8} E'(z(t))(z(t+h) - z(t-h)) + \dots \right) \right] \times B(z(t)) \\
& \quad + E(z(t)) + \frac{1}{4} E'(z(t)) [z(t+h) - 2z(t) + z(t-h)] + \dots.
\end{aligned}$$

Letting $z := z(t)$ and expanding the above functions in powers of h , we obtain

$$\begin{aligned}
\ddot{z} + \frac{h^2}{12} \dddot{z} + \dots &= \frac{\tan\left(\frac{h}{2}|B(z)|\right)}{\frac{h}{2}|B(z)|} \left[\left(\dot{z} + \frac{h^2}{6} \ddot{z} + \dots \right) - \left(\frac{h^2}{4} E'(z) \left(\dot{z} + \frac{h^2}{6} \ddot{z} + \dots \right) + \dots \right) \right] \times B(z) \\
& \quad + E(z) + \frac{h^2}{4} E'(z) \left(\ddot{z} + \frac{h^2}{12} \dddot{z} + \dots \right) + \dots.
\end{aligned} \tag{17}$$

We note that when $h = 0$, the equations (16) and (17) are both identical to (1). In fact, differentiating these two equations recursively and considering $h = 0$ shows that the third and higher derivatives depend on (z, \dot{z}) . Then we get a modified equation in even powers of h :

$$\ddot{z} = \frac{\tan\left(\frac{h}{2}|B(z)|\right)}{\frac{h}{2}|B(z)|} \dot{z} \times B(z) + E(z) + h^2 F_2(z, \dot{z}) + h^4 F_4(z, \dot{z}) + \dots,$$

where the coefficient functions depend on (z, \dot{z}) . By taking inner product on both sides of (16) and (17) with different expressions, we can prove Theorem 3.1–3.3 in the following three subsections, respectively.

4.2. Proof of the energy conservation (Theorem 3.1)

Since it has been shown in [24] that IMS-O2 is an energy-preserving method, here we just prove the exact conservation of modified energy and the long time behaviour of energy for EXS-O2. To prove the result, we need to derive two almost invariants which are close to the energy $H(x, v)$. The first one is deduced from the following lemma and the second is obtained with the help of Lemma 4.4.

Lemma 4.1. *It is obtained a function*

$$H_h(x, v) = H(x, v) + h^2 H_2(x, v) + h^4 H_4(x, v) + \dots$$

such that

$$\frac{d}{dt} H_h(z, \dot{z}) = \frac{\tan\left(\frac{h}{2} |B(z)|\right)}{\frac{h}{2} |B(z)|} \dot{z}^\top \left(\frac{h^2}{3!} \ddot{z} + \frac{h^4}{5!} z^{(5)} + \dots \right) \times B(z) + O(h^N)$$

along solutions of the modified differential equation (16), where the functions $H_{2j}(x, v)$ are independent of the step size h and $O(h^N)$ is the truncation term.

Proof. Multiplying (16) with \dot{z}^\top and using the fact that

$$\dot{z}^\top z^{(2k)} = \frac{d}{dt} \left(\dot{z}^\top z^{(2k-1)} - \ddot{z}^\top z^{(2k-2)} + \dots + \frac{(-1)^{k+1}}{2} (z^{(k)})^\top z^{(k)} \right),$$

we get

$$\frac{d}{dt} \left(\frac{1}{2} \dot{z}^\top \dot{z} + U(z) + \frac{h^2}{12} \left(\dot{z}^\top \ddot{z} - \frac{1}{2} \ddot{z}^\top \dot{z} \right) + \dots \right) = \frac{\tan\left(\frac{h}{2} |B(z)|\right)}{\frac{h}{2} |B(z)|} \dot{z}^\top \left(\frac{h^2}{3!} \ddot{z} + \frac{h^4}{5!} z^{(5)} + \dots \right) \times B(z) + O(h^N).$$

Then the result of this lemma is immediately obtained. \blacksquare

Corollary 4.2. *(The first almost invariant close to energy) If the magnetic field is constant, i.e., $B(x) \equiv B$, we have a function*

$$\tilde{H}_h(x, v) = H(x, v) + h^2 \tilde{H}_2(x, v) + h^4 \tilde{H}_4(x, v) + \dots$$

satisfying

$$\frac{d}{dt} \tilde{H}_h(z, \dot{z}) = O(h^N)$$

along solutions of the modified differential equation (16), where the functions $\tilde{H}_{2j}(x, v)$ are independent of h and $O(h^N)$ is the truncation term.

Proof. Based on the results in Lemma 4.1 and the fact that

$$\dot{z}^\top (z^{(2k+1)} \times B) = \frac{d}{dt} \left(\dot{z}^\top (z^{(2k)} \times B) - \ddot{z}^\top (z^{(2k-1)} \times B) + \dots + (-1)^{k+1} (z^{(k)})^\top (z^{(k+1)} \times B) \right),$$

the first statement is obtained. Then, it is arrived that

$$\frac{d}{dt} \left(\frac{1}{2} \dot{z}^\top \dot{z} + U(z) + \frac{h^2}{12} \left(\dot{z}^\top \ddot{z} - \frac{1}{2} \ddot{z}^\top \dot{z} \right) - \frac{\tan\left(\frac{h}{2} |B|\right)}{\frac{h}{2} |B|} \left(\frac{h^2}{3!} \dot{z}^\top (\ddot{z} \times B) + \dots \right) + \dots \right) = O(h^N),$$

which completes the proof. \blacksquare

Remark 4.3. It is noted that based on this corollary, the method EXS-O2 will be shown to have a long-time near-conservation of the energy for a constant magnetic field B .

Lemma 4.4. There exists a function

$$H_h(x, v) = H(x, v) + h^2 H_2(x, v) + h^4 H_4(x, v) + \dots$$

and it satisfies

$$\frac{d}{dt} H_h(z, \dot{z}) = \left(\frac{h^2}{3!} \ddot{z} + \frac{h^4}{5!} z^{(5)} + \dots \right)^\top E(z) + O(h^N)$$

along solutions obtained by the modified differential equation (16), where the functions $H_{2j}(x, v)$ (different from those in Lemma 4.1) don't depend on the step size h and $O(h^N)$ is the truncation term.

Proof. It is noted that if $l + m$ is odd, $z^{(l)\top} z^{(m)}$ can be written as a total differential. Then taking inner product on both sides of (16) with $\left(\dot{z} + \frac{h^2}{6} \ddot{z} + \dots \right)$ and using the same arguments of Lemma 4.1, one has

$$\frac{d}{dt} \left(\frac{1}{2} \dot{z}^\top \dot{z} + U(z) + \frac{h^2}{12} \left(\dot{z}^\top \ddot{z} - \frac{1}{2} \ddot{z}^\top \dot{z} \right) + \dots \right) = \left(\frac{h^2}{3!} \ddot{z} + \frac{h^4}{5!} z^{(5)} + \dots \right)^\top E(z) + O(h^N).$$

The proof is complete. ■

Corollary 4.5. (The second almost invariant close to energy) If $U(x) = \frac{1}{2} x^\top Q x + q^\top x$, we get a function

$$\widehat{H}_h(x, v) = H(x, v) + h^2 \widehat{H}_2(x, v) + h^4 \widehat{H}_4(x, v) + \dots$$

such that

$$\frac{d}{dt} \widehat{H}_h(z, \dot{z}) = O(h^N)$$

along solutions of the modified differential equation (16), where the functions $H_{2j}(x, v)$ are independent of h and $O(h^N)$ is the truncation term.

Proof. Since the expression $z^{(2k+1)\top} \nabla U(z) = z^{(2k+1)\top} (Qz + q)$ is a total differential:

$$\left(z^{(2k+1)} \right)^\top (Qz + q) = \frac{d}{dt} \left(\left(z^{(2k)} \right)^\top (Qz + q) - \left(z^{(2k-1)} \right)^\top Q \dot{z} + \dots + \frac{(-1)^k}{2} \left(z^{(k)} \right)^\top Q z^{(k)} \right),$$

it is clear that

$$\frac{d}{dt} \left(\frac{1}{2} \dot{z}^\top \dot{z} + U(z) + \frac{h^2}{12} \left(\dot{z}^\top \ddot{z} - \frac{1}{2} \ddot{z}^\top \dot{z} \right) + \frac{h^2}{6} \left(\ddot{z}^\top (Qz + q) - \frac{1}{2} \dot{z}^\top Q \dot{z} \right) + \dots \right) = O(h^N).$$

■

Remark 4.6. This result confirms that the method EXS-O2 hold a long-term near-conservation of the total energy as long as the scalar potential is quadratic.

Based on the above preparations, we are in the position to prove the results (10) and (12) of Theorem 3.1.

Proof of (10). The result is firstly shown for a constant magnetic field B . From Corollary 4.2, it follows that

$$\begin{aligned} H(x^n, v^n) &= \tilde{H}_h(x^n, v^n) + O(h^2) = \tilde{H}_h(x^0, v^0) + \sum_{k=1}^n (\tilde{H}_h(x^k, v^k) - \tilde{H}_h(x^{k-1}, v^{k-1})) + O(h^2) \\ &= H(x^0, v^0) + O(h^2) + nO(h^{N+1}) + O(h^2) = H(x^0, v^0) + O(h^2). \end{aligned} \quad (18)$$

The last equation is meaningful if and only if $nh^{N+1} \leq h^2$, i.e. $nh \leq h^{2-N}$ and this gives the desired bound for the deviation of the total energy along the numerical solution. Moreover, for the quadratic scalar potential, Corollary 4.5 implies $H(x^n, v^n) = \tilde{H}_h(x^n, v^n) + O(h^2)$. Using the same derivation as stated above, it is easy to show that the result (10) also holds for the quadratic scalar potential. ■

Proof of (12). The second equation in (9) can be reformulated as

$$e^{-\frac{h}{2}\tilde{B}(x^{n+1})}v^{n+1} = e^{\frac{h}{2}\tilde{B}(x^n)}v^n + \frac{h}{2}[E(x^n) + E(x^{n+1})].$$

This result and the fact that \tilde{B} is skew-symmetric imply

$$\begin{aligned} \frac{1}{2}(v^{n+1})^\top v^{n+1} - \frac{1}{2}(v^n)^\top v^n &= \frac{1}{2}(e^{-\frac{h}{2}\tilde{B}(x^{n+1})}v^{n+1})^\top (e^{-\frac{h}{2}\tilde{B}(x^{n+1})}v^{n+1}) - \frac{1}{2}(e^{\frac{h}{2}\tilde{B}(x^n)}v^n)^\top (e^{\frac{h}{2}\tilde{B}(x^n)}v^n) \\ &= \frac{1}{2}[E(x^n) + E(x^{n+1})]^\top \left[he^{\frac{h}{2}\tilde{B}(x^n)}v^n + \frac{h^2}{4}[E(x^n) + E(x^{n+1})] \right]. \end{aligned}$$

Besides, the deviation of U at x^{n+1} and x^n can be expressed as

$$\begin{aligned} U(x^{n+1}) - U(x^n) &= \frac{1}{2}(x^{n+1})^\top Qx^{n+1} + q^\top x^{n+1} - \left(\frac{1}{2}(x^n)^\top Qx^n + q^\top x^n \right) \\ &= \frac{1}{2}(x^{n+1} + x^n)^\top Q(x^{n+1} - x^n) + q^\top (x^{n+1} - x^n) \\ &= \left[\frac{1}{2}(x^{n+1} + x^n)^\top Q + q^\top \right] \left(he^{\frac{h}{2}\tilde{B}(x^n)}v^n + \frac{h^2}{2}E(x^n) \right). \end{aligned}$$

Therefore

$$\frac{1}{2}(v^{n+1})^\top v^{n+1} - \frac{1}{2}(v^n)^\top v^n + U(x^{n+1}) - U(x^n) = \frac{h^2}{8} |\nabla U(x^{n+1})|^2 - \frac{h^2}{8} |\nabla U(x^n)|^2$$

and this further gives $H_h(x^{n+1}, v^{n+1}) = H_h(x^n, v^n)$. ■

4.3. Proof of the momentum conservation (Theorem 3.2)

The proof is given by finding two almost invariants which are close to momentum. To derive these invariants, we first present the following lemma.

Lemma 4.7. *The following two functions*

$$\begin{aligned} M_h^e(x, v) &= M(x, v) + h^2 M_2^e(x, v) + h^4 M_4^e(x, v) + \cdots, \\ M_h^i(x, v) &= M(x, v) + h^2 M_2^i(x, v) + h^4 M_4^i(x, v) + \cdots, \end{aligned}$$

can be derived with the h -independent functions $M_{2j}^e(x, v)$ and $M_{2j}^i(x, v)$, and they satisfy

$$\frac{d}{dt} M_h^e(z, \dot{z}) = \frac{\tan\left(\frac{h}{2}|B(z)|\right)}{\frac{h}{2}|B(z)|} z^\top S \left(\frac{h^2}{3!} \ddot{z} + \frac{h^4}{5!} z^{(5)} + \dots \right) \times B(z) + O(h^N)$$

along solutions of the modified differential equation (16) for EXS-O2 and

$$\begin{aligned} \frac{d}{dt} M_h^i(z, \dot{z}) &= \frac{\tan\left(\frac{h}{2}|B(z)|\right)}{\frac{h}{2}|B(z)|} z^\top S \left[\left(\frac{h^2}{3!} \ddot{z} + \frac{h^4}{5!} z^{(5)} + \dots \right) - \frac{h^2}{4} E'(z) \left(\dot{z} + \frac{h^2}{3!} \ddot{z} + \dots \right) + \dots \right] \times B(y) \\ &\quad + \frac{h^2}{4} z^\top S E'(z) \left(\ddot{z} + \frac{h^2}{12} \ddot{z} + \dots \right) + \dots + O(h^N) \end{aligned}$$

along solutions of the modified differential equation (17) for IMS-O2.

Proof. We first multiply (16) and (17) with $\dot{z}^\top S$. Then notice the fact that the expression $z^\top S z^{(2k)}$ takes a form of total derivative:

$$z^\top S z^{(2k)} = \frac{d}{dt} \left(z^\top S z^{(2k-1)} - \dot{z}^\top S z^{(2k-2)} + \dots + (-1)^{k-1} \left(z^{(k-1)} \right)^\top S z^{(k)} \right).$$

In addition, the invariance properties (3) show that $z^\top S \nabla U(z) = 0$ and $z^\top S (\dot{z} \times B(z)) = -\frac{d}{dt} (z^\top S A(z))$ [12]. Based on the above results, we get

$$\begin{aligned} &\frac{d}{dt} \left(z^\top S \dot{z} + \frac{\tan\left(\frac{h}{2}|B(z)|\right)}{\frac{h}{2}|B(z)|} z^\top S A(z) + \frac{h^2}{12} (z^\top S \ddot{z} - \dot{z}^\top S \ddot{z}) + \dots \right) \\ &= \frac{\tan\left(\frac{h}{2}|B(z)|\right)}{\frac{h}{2}|B(z)|} z^\top S \left(\frac{h^2}{3!} \ddot{z} + \frac{h^4}{5!} z^{(5)} + \dots \right) \times B(z) + O(h^N) \end{aligned}$$

and by expansion of $\frac{\tan x}{x}$, the above equation can be rewritten as

$$\begin{aligned} &\frac{d}{dt} \left(z^\top S \dot{z} + z^\top S A(z) + \frac{h^2}{3} \left(\frac{|B(z)|}{2} \right)^2 z^\top S A(z) + \frac{h^2}{12} (z^\top S \ddot{z} - \dot{z}^\top S \ddot{z}) + \dots \right) \\ &= \frac{\tan\left(\frac{h}{2}|B(z)|\right)}{\frac{h}{2}|B(z)|} z^\top S \left(\frac{h^2}{3!} \ddot{z} + \frac{h^4}{5!} z^{(5)} + \dots \right) \times B(z) + O(h^N) \end{aligned}$$

for EXS-O2.

Similarly, we can get

$$\begin{aligned} &\frac{d}{dt} \left(z^\top S \dot{z} + z^\top S A(z) + \frac{h^2}{3} \left(\frac{|B(z)|}{2} \right)^2 z^\top S A(z) + \frac{h^2}{12} (z^\top S \ddot{z} - \dot{z}^\top S \ddot{z}) + \dots \right) \\ &= \frac{\tan\left(\frac{h}{2}|B(z)|\right)}{\frac{h}{2}|B(z)|} z^\top S \left[\left(\frac{h^2}{3!} \ddot{z} + \frac{h^4}{5!} z^{(5)} + \dots \right) - \frac{h^2}{4} E'(z) \left(\dot{z} + \frac{h^2}{3!} \ddot{z} + \dots \right) + \dots \right] \times B(z) \\ &\quad + \frac{h^2}{4} z^\top S E'(z) \left(\ddot{z} + \frac{h^2}{12} \ddot{z} + \dots \right) + \dots + O(h^N) \end{aligned}$$

for IMS-O2. ■

The above results can be improved under some conditions, which is stated by the following corollary.

Corollary 4.8. (The first almost invariant close to momentum) *If $B(x) \equiv B$ and $x^\top \nabla U(x) \times B = 0$ for all x , it is obtained that the functions*

$$\widehat{M}_h^e(x, v) = M(x, v) + h^2 \widehat{M}_2^e(x, v) + h^4 \widehat{M}_4^e(x, v) + \dots,$$

$$\widehat{M}_h^i(x, v) = M(x, v) + h^2 \widehat{M}_2^i(x, v) + h^4 \widehat{M}_4^i(x, v) + \dots,$$

satisfy

$$\frac{d}{dt} \widehat{M}_h^e(z, \dot{z}) = O(h^N)$$

along solutions of the modified differential equation (16) for EXS-O2 and

$$\begin{aligned} \frac{d}{dt} \widehat{M}_h^i(z, \dot{z}) &= \frac{\tan\left(\frac{h}{2} |B(z)|\right)}{\frac{h}{2} |B(z)|} z^\top S \left[-\frac{h^2}{4} E'(z) \left(\dot{z} + \frac{h^2}{6} \ddot{z} + \dots \right) + \dots \right] \times B(z) \\ &\quad + \frac{h^2}{4} z^\top S E'(z) \left(\ddot{z} + \frac{h^2}{12} \dddot{z} + \dots \right) + \dots + O(h^N) \end{aligned}$$

along solutions of the modified differential equation (17) for IMS-O2. Here the functions $\widehat{M}_{2j}^e(x, v)$ and $\widehat{M}_{2j}^i(x, v)$ are h -independent and $O(h^N)$ is the truncation term.

Proof. Using the same way as that of Lemma 4.7 and noticing that $z^\top S(z^{(2k+1)} \times B)$ is a total derivative (due to the symmetry of S^2):

$$z^\top S(z^{(2k+1)} \times B) = z^\top S^2 z^{(2k+1)} = \frac{d}{dt} \left(z^\top S^2 z^{(2k)} - \dot{z}^\top S^2 z^{(2k-1)} + \dots + \frac{(-1)^k}{2} (z^{(k)})^\top S^2 z^{(k)} \right),$$

we get

$$\begin{aligned} &\frac{d}{dt} \left(z^\top S \dot{z} + z^\top S A(z) + \frac{h^2}{3} \left(\frac{|B|}{2} \right)^2 z^\top S A(z) + \frac{h^2}{12} (z^\top S \ddot{z} - \dot{z}^\top S \dot{z}) - \frac{h^2 \tan\left(\frac{h}{2} |B|\right)}{6 \frac{h}{2} |B|} \left(z^\top S^2 \ddot{z} - \frac{1}{2} \dot{z}^\top S^2 \dot{z} \right) + \dots \right) \\ &= O(h^N) \end{aligned}$$

for EXS-O2 and

$$\begin{aligned} &\frac{d}{dt} \left(z^\top S \dot{z} + z^\top S A(z) + \frac{h^2}{3} \left(\frac{|B|}{2} \right)^2 z^\top S A(z) + \frac{h^2}{12} (z^\top S \ddot{z} - \dot{z}^\top S \dot{z}) - \frac{h^2 \tan\left(\frac{h}{2} |B|\right)}{6 \frac{h}{2} |B|} \left(z^\top S^2 \ddot{z} - \frac{1}{2} \dot{z}^\top S^2 \dot{z} \right) + \dots \right) \\ &= \frac{\tan\left(\frac{h}{2} |B|\right)}{\frac{h}{2} |B|} z^\top S \left[-\frac{h^2}{4} E'(z) \left(\dot{z} + \frac{h^2}{6} \ddot{z} + \dots \right) + \dots \right] \times B + \frac{h^2}{4} z^\top S E'(z) \left(\ddot{z} + \frac{h^2}{12} \dddot{z} + \dots \right) + \dots + O(h^N) \end{aligned} \tag{19}$$

for IMS-O2. ■

Corollary 4.9. (The second almost invariant close to momentum) Suppose that the conditions in Corollary 4.8 are satisfied and $U(x) = \frac{1}{2}x^\top Qx + q^\top x$ with $QS = S^\top Q$. Then the function

$$\tilde{M}_h^i(x, v) = M(x, v) + h^2 \tilde{M}_2^i(x, v) + h^4 \tilde{M}_4^i(x, v) + \dots$$

satisfies

$$\frac{d}{dt} \tilde{M}_h^i(z, \dot{z}) = O(h^N)$$

along solutions of the modified differential equation (17) for IMS-O2. Here the functions $\tilde{M}_{2j}^i(x, v)$ don't depend on the step size h and $O(h^N)$ stands for the truncation term.

Proof. Based on the assumptions, the right-hand side of (19) can be simplified as

$$\begin{aligned} & \frac{\tan\left(\frac{h}{2}|B|\right)}{\frac{h}{2}|B|} z^\top S \left[-\frac{h^2}{4} E'(z) \left(\dot{z} + \frac{h^2}{6} \ddot{z} + \dots \right) + \dots \right] \times B + \frac{h^2}{4} z^\top S E'(z) \left(\ddot{z} + \frac{h^2}{12} \dddot{z} + \dots \right) + \dots + O(h^N) \\ &= \frac{\tan\left(\frac{h}{2}|B|\right)}{\frac{h}{2}|B|} z^\top S \left[\frac{h^2}{4} Q \left(\dot{z} + \frac{h^2}{6} \ddot{z} + \dots \right) \right] \times B - \frac{h^2}{4} z^\top S Q \left(\ddot{z} + \frac{h^2}{12} \dddot{z} + \dots \right) + O(h^N). \end{aligned}$$

According to the properties of S and Q , it is obtained that SQ is skew-symmetric and S^2Q is symmetric. Then, we get

$$z^\top S \left((Qz^{(2k+1)}) \times B \right) = z^\top S^2 Qz^{(2k+1)} = \frac{d}{dt} \left(z^\top S^2 Qz^{(2k)} - \dot{z}^\top S^2 Qz^{(2k-1)} + \dots + \frac{(-1)^k}{2} (z^{(k)})^\top S^2 Qz^{(k)} \right)$$

and

$$z^\top S Qz^{(2k)} = \frac{d}{dt} \left(z^\top S Qz^{(2k-1)} - \dot{z}^\top S Qz^{(2k-2)} + \dots + (-1)^{k-1} (z^{(k-1)})^\top S Qz^{(k)} \right).$$

Therefore, the proof is complete. ■

Proof of (13). With the results stated above, the method EXS-O2 conserves the momentum with the accuracy

$$\begin{aligned} M(x^n, v^n) &= \tilde{M}_h^e(x^n, v^n) + O(h^2) = \tilde{M}_h^e(x^0, v^0) + \sum_{k=1}^n \left(\tilde{M}_h^e(x^k, v^k) - \tilde{M}_h^e(x^{k-1}, v^{k-1}) \right) + O(h^2) \\ &= M(x^0, v^0) + O(h^2) + nO(h^{N+1}) + O(h^2) = M(x^0, v^0) + O(h^2), \end{aligned} \tag{20}$$

as long as $nh \leq h^{2-N}$. For IMS-O2, the same discussion applies to $\tilde{M}_h^i(x, v)$ and then (13) can be proved. ■

4.4. Proof of the magnetic moment conservation (Theorem 3.3)

In this section, we just considered magnetic moment in constant magnetic field B , that is

$$I(x, v) = \frac{|v \times B|^2}{2|B|^3} = \frac{|v \times b|^2}{2|B|}$$

with $b = \frac{B}{|B|}$ and a skew-symmetric matrix $\widehat{B} = \frac{\widehat{B}}{|B|}$ satisfying $v \times b = \widehat{B}v$.

Specifically, the modified equations (16) and (17) are respectively equivalent to

$$\left(\dot{z} + \frac{h^2}{6}\ddot{z} + \dots\right) \times b = \frac{h}{2 \tan\left(\frac{h}{2}|B|\right)} \left[\left(\ddot{z} + \frac{h^2}{12}\dddot{z} + \dots\right) - E(z)\right] \quad (21)$$

and

$$\begin{aligned} \left(\dot{z} + \frac{h^2}{6}\ddot{z} + \dots\right) \times b = & \frac{h}{2 \tan\left(\frac{h}{2}|B|\right)} \left[\left(\ddot{z} + \frac{h^2}{12}\dddot{z} + \dots\right) - \left(E(z) + \frac{h^2}{4}E'(z)\left(\ddot{z} + \frac{h^2}{12}\dddot{z} + \dots\right) + \dots\right)\right] \\ & + \left(\frac{h^2}{4}E'(z)\left(\dot{z} + \frac{h^2}{6}\ddot{z} + \dots\right) + \dots\right) \times b. \end{aligned} \quad (22)$$

Based on these results, we can derive two almost invariants close to magnetic moment, which will complete the proof of Theorem 3.3. To this end, we first prove the following result.

Lemma 4.10. *If $B(x) \equiv B$, one gets that the functions*

$$I_h^e(x, v) = I(x, v) + h^2 I_2^e(x, v) + h^4 I_4^e(x, v) + \dots,$$

$$I_h^i(x, v) = I(x, v) + h^2 I_2^i(x, v) + h^4 I_4^i(x, v) + \dots,$$

satisfy

$$\frac{d}{dt} I_h^e(z, \dot{z}) = -\frac{h}{2|B| \tan\left(\frac{h}{2}|B|\right)} (\ddot{z} \times b)^\top E(z) + O(h^N)$$

along solutions of the modified differential equation (16) for EXS-O2 and

$$\begin{aligned} \frac{d}{dt} I_h^i(z, \dot{z}) = & -\frac{h}{2|B| \tan\left(\frac{h}{2}|B|\right)} (\ddot{z} \times b)^\top \left[E(z) + \frac{h^2}{4}E'(z)\left(\ddot{z} + \frac{h^2}{12}\dddot{z} + \dots\right) + \dots\right] \\ & + \frac{1}{|B|} (\ddot{z} \times b)^\top \left[\frac{h^2}{4}E'(z)\left(\dot{z} + \frac{h^2}{6}\ddot{z} + \dots\right) + \dots\right] \times b + O(h^N) \end{aligned}$$

along solutions of the modified differential equation (17) for IMS-O2. Here the functions $I_{2,j}^e(x, v)$ and $I_{2,j}^i(x, v)$ are h -independent and $O(h^N)$ is the truncation term.

Proof. Multiply (21) and (22) with $\frac{1}{|B|}(\ddot{z} \times b)^\top$. It is clear that

$$\begin{aligned} & \frac{1}{|B|} (\ddot{z} \times b)^\top \left(\dot{z}^{(2k+1)} \times b\right) \\ &= \begin{cases} \frac{d}{dt} I(z, \dot{z}), & k = 0 \\ \frac{d}{dt} \frac{1}{|B|} \left((\ddot{z} \times b)^\top \left(\dot{z}^{(2k)} \times b\right) - (\ddot{z} \times b)^\top \left(\dot{z}^{(2k-1)} \times b\right) + \dots + \frac{(-1)^{k+1}}{2} \left(\dot{z}^{(k+1)} \times b\right)^\top \left(\dot{z}^{(k+1)} \times b\right)\right), & k \in \mathbb{N}^* \end{cases} \end{aligned}$$

and

$$\begin{aligned} & \frac{1}{|B|} (\ddot{z} \times b)^\top \dot{z}^{(2k)} \\ &= \begin{cases} 0, & k = 1 \\ \frac{d}{dt} \frac{1}{|B|} \left((\ddot{z} \times b)^\top \dot{z}^{(2k-1)} - (\ddot{z} \times b)^\top \dot{z}^{(2k-2)} + \dots + (-1)^k \left(\dot{z}^{(k)} \times b\right)^\top \dot{z}^{(k+1)}\right), & k \in \mathbb{N}^* - \{1\} \end{cases} \end{aligned}$$

These immediately demonstrate that

$$\begin{aligned} & \frac{d}{dt} \left[I(z, \dot{z}) + \frac{h^2}{12|B|} (\ddot{z} \times b)^\top (\ddot{z} \times b) - \frac{h}{2|B| \tan\left(\frac{h}{2}|B|\right)} \left(\frac{h^2}{12} (\ddot{z} \times b)^\top \ddot{\ddot{z}} + \dots \right) \right] \\ &= -\frac{h}{2|B| \tan\left(\frac{h}{2}|B|\right)} (\ddot{z} \times b)^\top E(z) + O(h^N) \end{aligned}$$

for EXS-O2.

On the other hand and with the same arguments, we get

$$\begin{aligned} & \frac{d}{dt} \left[I(z, \dot{z}) + \frac{h^2}{12|B|} (\ddot{z} \times b)^\top (\ddot{z} \times b) - \frac{h}{2|B| \tan\left(\frac{h}{2}|B|\right)} \left(\frac{h^2}{12} (\ddot{z} \times b)^\top \ddot{\ddot{z}} + \dots \right) \right] \\ &= -\frac{h}{2|B| \tan\left(\frac{h}{2}|B|\right)} (\ddot{z} \times b)^\top \left[E(z) + \frac{h^2}{4} E'(z) \left(\ddot{z} + \frac{h^2}{12} \ddot{\ddot{z}} + \dots \right) + \dots \right] \\ &+ \frac{1}{|B|} (\ddot{z} \times b)^\top \left[\frac{h^2}{4} E'(z) \left(\dot{z} + \frac{h^2}{6} \ddot{\ddot{z}} + \dots \right) + \dots \right] \times b + O(h^N) \end{aligned} \quad (23)$$

for IMS-O2. ■

Corollary 4.11. (*The almost invariants close to magnetic moment*) If $B(x) \equiv B$ and $U(x) = \frac{1}{2}x^\top Qx + q^\top x$ with $QB = \bar{B}Q$, one obtains that the functions

$$\begin{aligned} \widehat{I}_h^e(x, v) &= I(x, v) + h^2 \widehat{I}_2^e(x, v) + h^4 \widehat{I}_4^e(x, v) + \dots, \\ \widehat{I}_h^i(x, v) &= I(x, v) + h^2 \widehat{I}_2^i(x, v) + h^4 \widehat{I}_4^i(x, v) + \dots, \end{aligned}$$

satisfy

$$\frac{d}{dt} \widehat{I}_h^e(z, \dot{z}) = O(h^N)$$

along solutions of the modified differential equation (16) for EXS-O2, and

$$\frac{d}{dt} \widehat{I}_h^i(z, \dot{z}) = O(h^N)$$

along solutions of the modified differential equation (17) for IMS-O2. Here the functions $\widehat{I}_{2j}^e(x, v)$ and $\widehat{I}_{2j}^i(x, v)$ are h -independent and $O(h^N)$ refers to the truncation term.

Proof. On the basis of the conditions above, $-(\ddot{z} \times b)^\top E(z) = (\ddot{z} \times b)^\top (Qz + q) = \frac{d}{dt} ((\ddot{z} \times b)^\top (Qz + q))$. The hand-side of (23) can be written as

$$\begin{aligned} & \frac{h}{2|B| \tan\left(\frac{h}{2}|B|\right)} (\ddot{z} \times b)^\top \left[(Qz + q) + \frac{h^2}{4} Q \left(\ddot{z} + \frac{h^2}{12} \ddot{\ddot{z}} + \dots \right) \right] \\ & - \frac{1}{|B|} (\ddot{z} \times b)^\top \left[\frac{h^2}{4} Q \left(\dot{z} + \frac{h^2}{6} \ddot{\ddot{z}} + \dots \right) \right] \times b + O(h^N). \end{aligned}$$

Since $\widehat{B}Q$ is skew-symmetric and \widehat{B}^2Q is symmetric, we have

$$\begin{aligned} & (\ddot{z} \times b)^\top Qz^{(2k)} \\ &= -\ddot{z}^\top \widehat{B}Qz^{(2k)} = \begin{cases} 0, & k = 1 \\ -\frac{d}{dt} \left(\ddot{z}^\top \widehat{B}Qz^{(2k-1)} - \ddot{\ddot{z}}^\top \widehat{B}Qz^{(2k-1)} + \dots + (-1)^k \left(z^{(k)} \right)^\top \widehat{B}Qz^{(k+1)} \right), & k \in \mathbb{N}^* - \{1\} \end{cases} \end{aligned}$$

and

$$\begin{aligned} & (\ddot{z} \times b)^\top (Qz^{(2k+1)}) \times b \\ &= -\ddot{z}^\top \widehat{B}^2Qz^{(2k+1)} = \begin{cases} -\frac{1}{2} \ddot{z}^\top \widehat{B}^2Q\dot{z}, & k = 0 \\ -\frac{d}{dt} \left(\ddot{z}^\top \widehat{B}^2Qz^{(2k)} - \ddot{\ddot{z}}^\top \widehat{B}^2Qz^{(2k-1)} + \dots + \frac{(-1)^{k+1}}{2} \left(z^{(k+1)} \right)^\top \widehat{B}^2Qz^{(k+1)} \right), & k \in \mathbb{N}^*. \end{cases} \end{aligned}$$

For the sake of formal unity, we formulate $-\ddot{z}^{(l)\top} \widehat{B}^2Qz^{(m)}$ as $\left(z^{(l)} \times b \right)^\top (Qz^{(m)}) \times b$ for any integers l and m . Hence,

$$\frac{d}{dt} \left[I(z, \dot{z}) + \frac{h^2}{12|B|} (\ddot{z} \times b)^\top (\ddot{z} \times b) - \frac{h}{2|B|\tan\left(\frac{h}{2}|B|\right)} \left(\left(\frac{h^2}{12} (\ddot{z} \times b)^\top \ddot{\ddot{z}} + \dots \right) + (\dot{z} \times b)^\top (Qz + q) \right) \right] = O(h^N)$$

along solutions of the modified differential equation (16) for EXS-O2, and

$$\begin{aligned} & \frac{d}{dt} \left[I(z, \dot{z}) + \frac{h^2}{12|B|} (\ddot{z} \times b)^\top (\ddot{z} \times b) - \frac{h}{2|B|\tan\left(\frac{h}{2}|B|\right)} \left(\frac{h^2}{12} (\ddot{z} \times b)^\top \ddot{\ddot{z}} + \dots \right) \right] \\ & - \frac{d}{dt} \left[\frac{h}{2|B|\tan\left(\frac{h}{2}|B|\right)} \left((\ddot{z} \times b)^\top (Qz + q) + \frac{h^2}{4} \left(\frac{h^2}{12} (\ddot{z} \times b)^\top Q\ddot{\ddot{z}} + \dots \right) \right) \right] \\ & + \frac{d}{dt} \left[\frac{h^2}{4|B|} \left(\frac{1}{2} (\dot{z} \times b)^\top (Q\dot{z}) \times b + \dots \right) \right] = O(h^N). \end{aligned}$$

■

Proof of (14). The proof of (14) is the same as that of (10) and (13), and we omit it for brevity. ■

5. Conclusion

In this paper, we presented two splitting algorithms and studied their long-term behaviour for solving charged-particle dynamics. Using backward error analysis, it was shown that these two algorithms have good conservations of energy, momentum and magnetic moment in some special cases. Furthermore, one algorithm was proved to conserve a modified energy exactly. All the results were illustrated by some numerical tests.

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